Polymer state approximation of Schrödinger wave functions

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Abstract

It is shown how states of a quantum mechanical particle in the Schrödinger representation can be approximated by states in the so-called polymer representation. The result may shed some light on the semiclassical limit of loop quantum gravity.

1 Introduction

A fundamental feature of the algebraic formulation of quantum physics is the fact, that the states of any faithful representation of a C*-algebra form a $*$-weakly dense subset of the full state space of the algebra (Fell' s Theorem)(see e.g. [3, 4]). This general fact becomes relevant if one tries to compare states in the so-called polymer representations of loop quantum gravity with states occuring in quantum field theory. It is a highly debated question whether loop quantum gravity has the potential to describe continuum physics in an appropriate limit (see, e.g. [5]-[10]). A toy model for which this question can be discussed is provided by quantum mechanics of a single particle in 1 spatial dimension (see [1, 5]). This model also has direct relevance for cosmological considerations (see [11]).

Whereas the critics of the principal possibility to approximate states in the standard Schrödinger representation by states in a singular representation of the canonical commutation relations is unjustified in view of Fell's

Theorem, the answers in the affirmative given so far (see [1]) are not completely satisfactory. Namely, in this paper, expectation values in some state in the Schrödinger representation are approximated by linear functionals obtained by pairing vectors in a dense subspace of the representation space of the polymer representation (called the subspace of cylindrical functions) with elements of the dual. One would like to interpret these functionals as expectation values of state vectors in the polymer representation. But they are neither normal with respect to the polymer representation (e.g. a sequence of Weyl operators may converge weakly to zero in the polymer representation, but their values in these functionals may approach a finite value) nor are they positive. On the other hand, the answer via Fell's Theorem suffers from the fact that the theorem does not give an explicit construction of the approximating states (it is based on the Hahn-Banach Theorem). We therefore aim in this note at closing these gaps.

2 Weyl algebra and polymer representation

In the Schrödinger representation, the Weyl operators

$$W(\alpha,\beta) := e^{i(\alpha q+\beta p)} \tag{1}$$

with the standard momentum and position operators p and q and $\alpha,\beta\in\mathbb{R}$, satisfy the Weyl relation

$$W(\alpha_1,\beta_1)W(\alpha_2,\beta_2) = e^{-\frac{i}{2}(\alpha_1\beta_2-\alpha_2\beta_1)}W(\alpha_1+\alpha_2,\beta_1+\beta_2)\ . \tag{2}$$

Together with the unitarity condition

$$W(\alpha,\beta)^* = W(-\alpha,-\beta) \tag{3}$$

these relations alone define a unique simple C*-algebra, the Weyl algebra. The Schrödinger representation is (up to unitary equivalence) the only irreducible representation of the Weyl algebra in which the Weyl operators are continuous functions of α and β (with respect to the weak operator topology).

There are many irreducible representations where this continuity condition is not satisfied. One special example is the so-called polymer representation. The Hilbert space $\mathfrak{H}_{\text{poly}}$ in this representation consists of functions

Ψ on the real line which vanish up to a countable subset and satisfy the condition

$$\sum_{x\in\mathbb{R}} |\Psi(x)|^2 < \infty \ , \tag{4}$$

and the scalar product is defined by

$$(\Psi, \Phi) = \sum_{x\in\mathbb{R}} \overline{\Psi(x)}\Phi(x) \ . \tag{5}$$

The Weyl operators act on these functions in the same way as in the Schrödinger representation,[1]

$$(W(\alpha,\beta)\Psi)(x) = e^{-\frac{i}{2}\alpha\beta} e^{i\alpha x}\Psi(x-\beta) \ . \tag{6}$$

The position operator may be defined as usual on a dense subspace and possesses even a complete set of (normalizable) eigenvectors $\{|x\rangle, x \in \mathbb{R}\}$; the momentum operator, however, cannot be defined.

This well known representation shares some similarities with the so-called polymer representations in Loop Quantum Gravity and may serve as a toy model for the discussion of structural problems. In [1] the question was discussed in which way states in the Schrödinger representation can be approximated from the polymer representation. An inductive system of countable subsets M of $\mathbb{R}$ was found which has the property that for Schwartz space functions ψ the restriction to any of these subsets M defines an element $P_M\psi$ of the polymer Hilbert space. Every such wave function defines a linear functional on the inductive limit of the corresponding subspaces, called the space of cylindrical functions. We will denote this functional by $\langle\psi|$ and write its action on a state vector Φ as $\langle\psi|\Phi\rangle$. This action is defined by

$$\langle\psi|\Phi\rangle = (P_S\psi, \Phi) \ , \qquad \text{where} \qquad S = \text{supp}\,\Phi. \tag{7}$$

In order to define expectation values, the set M was specified to be a lattice of the form $\varepsilon\mathbb{Z}$. The expectation value in the state ψ was then approximated by

$$\varepsilon\,\langle\psi|AP_M\psi\rangle \ , \tag{8}$$

[1]To keep the notation simple we will use the same symbol for a Weyl operator in both representations. There will be no ambiguities since we denote state vectors in the Schrödinger Hilbert space by lower case greek letters and state vectors in $\mathfrak{H}_{\text{poly}}$ by capital greek letters.

where A is a finite linear combination of Weyl operators. Clearly, in the limit $\varepsilon \to 0$ the above expression converges to the expectation value in the Schrödinger representation.

Unfortunately, as already mentioned in the introduction, the approximation above cannot be understood as an approximation of Schrödinger states by polymer states in the sense of expectation values. First of all, the linear functional

$$A \to \varepsilon \langle \psi | A P_M \psi \rangle \tag{9}$$

is not normal with respect to the polymer representation, hence cannot be described in terms of matrix elements in this representation. Namely, consider the sequence $W(0, \frac{1}{n})$, $n \in \mathbb{N}$. Its matrix elements between arbitrary position eigenstates tend to zero, hence, being a bounded sequence, it will converge to zero in the weak operator topology. On the other hand, in the linear functional above, we find

$$\varepsilon \sum_{z \in \mathbb{Z}} \overline{\psi(\varepsilon z + \tfrac{1}{n})} \psi(\varepsilon z) \to \varepsilon \sum_{z \in \mathbb{Z}} |\psi(\varepsilon z)|^2 \ . \tag{10}$$

The second problem is, that these functionals are not positive. Namely, choose

$$\psi(x) = e^{i\beta x} e^{-\frac{x^2}{2}} \tag{11}$$

as the Schrödinger wave function to be approximated. Choose $M = \varepsilon(\mathbb{Z} + \lambda)$ as a countable subset of the real line and the so-called shadow state

$$P_M \psi = \sum_{x \in M} \psi(x) |x\rangle \tag{12}$$

We compute the approximate expectation value of the positive operator

$$A = (1 - V(\alpha))^*(1 - V(\alpha)) = 2 - V(\alpha) - V(-\alpha) \ . \tag{13}$$

where $V(\alpha) = W(0, \alpha)$. We obtain

$$\varepsilon \langle \psi | (2 - (V(\alpha) + V(-\alpha)) P_M \psi \rangle = \tag{14}$$

$$\varepsilon \sum_{x \in M} (2|\psi(x)|^2 - (\overline{\psi(x + \alpha) + \psi(x - \alpha)}) \psi(x)) = \tag{15}$$

$$\varepsilon \sum_{x \in M} 2e^{-x^2} (1 - (\cosh \alpha x \cos \alpha\beta - i \sinh \alpha x \sin \alpha\beta) e^{-\frac{\alpha^2}{2}}) \tag{16}$$

which, in general, is not real.

3 Approximation by polymer states

Let $\psi \in L^2(\mathbb{R})$ be a normalized wave function in the Schrödinger representation. Let $A = (A_1, \ldots, A_n)$ be a finite number of elements of the Weyl algebra and let $\varepsilon = (\varepsilon_1, \ldots, \varepsilon_n)$ be a family of positive numbers. We search for a unit vector Ψ in the polymer representation such that

$$|(\psi, A_i\psi) - (\Psi, A_i\Psi)| < \varepsilon_i \ , \ i = 1, \ldots, n \tag{17}$$

We may find Weyl operators $W(\alpha_{ik}, \beta_{ik})$, $k = 1, \ldots N_i$, complex numbers λ_{ik}, such that

$$||A_i - \sum_k \lambda_{ik} W(\alpha_{ik}, \beta_{ik})|| < \frac{\varepsilon_i}{3} \tag{18}$$

We therefore may look for a vector Ψ, such that

$$|(\psi, W(\alpha_{ik}, \beta_{ik})\psi) - (\Psi, W(\alpha_{ik}, \beta_{ik})\Psi)| < \delta_{ik} \tag{19}$$

with $\sum_k |\lambda_{ik}|\delta_{ik} < \frac{\varepsilon_i}{3}$.

The expectation value in the Schrödinger representation has the form

$$(\psi, W(\alpha, \beta)\psi) = \int dx \, \overline{\psi(x)} e^{i\alpha(x+\frac{1}{2}\beta)} \psi(x - \beta) \ . \tag{20}$$

In the polymer representation we have instead

$$(\Psi, W(\alpha, \beta)\Psi) = \sum_{x\in\mathbb{R}} \overline{\Psi(x)} e^{i\alpha(x+\frac{1}{2}\beta)} \Psi(x - \beta) \ . \tag{21}$$

Therefore one might try to choose Ψ such that the latter sum is a Riemann approximation to the integral above. But for Ψ normalizable, the coefficients $\Psi(x)$ can be different from zero only on a countable subset supp $\Psi \subset \mathbb{R}$. Then the sum extends only over x in the intersection supp $\Psi \cap$supp $\Psi + \beta$. To ensure that the intersection is sufficiently large, one may choose a countable subset which is invariant under translation by β_n, $n = 1, \ldots, N$. But in the generic case such a set is dense in $\mathbb{R}$, hence the coefficients $\Psi(x)$ can not be identified with the values of the wave function $\psi(x)$, multiplied by the square root of the length of an appropriate interval.

Instead we may look at the additive subgroup of $\mathbb{R}$ which is generated by β_n, $n = 1, \ldots, N$. This subgroup is a torsion free abelian group and therefore isomorphic to $\mathbb{Z}^L$ for some $L \leq N$. The isomorphism Γ may be considered as the projection which maps the lattice $\mathbb{Z}^L$ onto a quasilattice in $\mathbb{R}$. It has a unique extension to a linear map from $\mathbb{R}^L$ onto $\mathbb{R}$ which we will denote by γ. γ may be identified with an element of $\mathbb{R}^L$ such that $\gamma(z) = \sum_i \gamma_i z_i$. We now choose a function χ of one real variable which is continuous, has compact support and satisfies the normalization condition

$$\int_{\mathbb{R}^{L-1}} dz^{L-1} |\chi(|z|^2)|^2 = 1 \tag{22}$$

where $|z|^2 = \sum_i z_i^2$. We approximate ψ within $L^2(\mathbb{R})$ by a continuous function ϕ with compact support and define a function ϕ_χ on $\mathbb{R}^L$ by

$$\phi_\chi(z) = |\gamma|^{\frac{L}{2}} \phi(\gamma(z)) \chi(|\gamma|^2|z|^2 - \gamma(z)^2) \ . \tag{23}$$

We then define approximating vectors $\Psi_{m,\chi}$, $m \in \mathbb{N}$ in the polymer space by

$$\Psi_{m,\chi} = m^{-\frac{L}{2}} \sum_{z \in \frac{1}{m}\mathbb{Z}^L} \phi_\chi(z) |\gamma(z)\rangle \ . \tag{24}$$

Inserting this into the formula for the expectation value we obtain

$$(\Psi_{m,\chi}, W(\alpha_n, \beta_n)\Psi_{m,\chi}) = m^{-L} \sum_{z \in \frac{1}{m}\mathbb{Z}^L} \overline{\phi_\chi(z)} e^{i\alpha_n(\gamma(z)+\frac{1}{2}\beta_n)} \phi_\chi(z - \Gamma^{-1}(\beta_n)) \ . \tag{25}$$

The latter expression is a Riemann approximation of the corresponding integral and will converge as m tends to infinity. The limit, however, will depend on the choice of χ. We obtain

$$\begin{aligned}\lim_{m\to\infty} (\Psi_{m,\chi}, W(\alpha_n, \beta_n)\Psi_{m,\chi}) &= \int d^L z \, \overline{\phi_\chi(z)} e^{i\alpha_n(\gamma(z)+\frac{1}{2}\beta_n)} \phi_\chi(z - \Gamma^{-1}(\beta_n)) \\ &= (\phi, W(\alpha_n, \beta_n)\phi) \int_{\gamma(z)=0} d^{L-1} z \, \overline{\chi(|z|^2)} \chi(|z - |\gamma|\Gamma^{-1}(\beta_n)|^2 - \beta_n^2)\end{aligned}$$

where, with an appropriate choice of coordinates, we separated the integral in the first line and obtained the expectation value in the state vector ϕ multiplied with an (L–1)-dimensional integral over the kernel of the function γ. Finally, in the last step, we choose χ such that the integral in the second line approaches unity. We may, e.g., scale χ by setting

$$\chi_\lambda(|z|^2) = \lambda^{\frac{L-1}{2}} \chi(\lambda^2 |z|^2) \ , \tag{26}$$

get

$$\int_{\gamma(z)=0} d^{L-1}z\, \overline{\chi_\lambda(|z|^2)}\chi_\lambda(|z-|\gamma|\Gamma^{-1}(\beta_n)|^2-\beta_n^2) =$$
$$\int_{\gamma(z)=0} d^{L-1}z\, \overline{\chi(|z|^2)}\chi(|z-\lambda|\gamma|\Gamma^{-1}(\beta_n)|^2-\lambda^2\beta_n^2)$$

and perform the limit $\lambda \to 0$.

3.1 Example

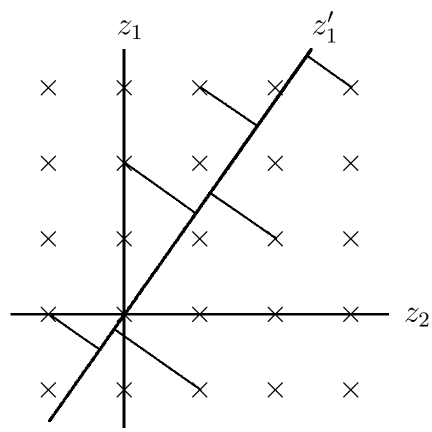
As an example of this method consider the simple case where the additive subgroup of $\mathbb{R}$ is generated by $\beta_1 = 1$ and $\beta_2 = \sqrt{2}$. The map $\Gamma(z) = \sum_i \beta_i z_i$ is then already an isomorphism. For the function ϕ_χ one gets

$$\phi_\chi(z) = \sqrt{3}\,\phi(z_1 + \sqrt{2}\,z_2)\,\chi(2z_1^2 + z_2^2 - 2\sqrt{2}\,z_1 z_2)\ . \tag{27}$$

One can introduce new coordinates z_1', z_2' defined by

$$\begin{aligned} z_1' &= z_1 + \sqrt{2}\,z_2\ , \\ z_2' &= \sqrt{2}\,z_1 - z_2\ . \end{aligned} \tag{28}$$

This corresponds to a rotation of the coordinate system such that the z_1'-axis now points in the direction defined by the vector $\beta = (\beta_1, \beta_2)$ in the old coordinates. The isomorphism Γ projects the points of $\mathbb{Z}^2$ onto the z_1'-axis. This is illustrated in the picture.



With these new coordinates the approximating vector in the polymer space has the form

$$\Psi_{m,\chi} = m^{-1} \sum_{z \in \frac{1}{m}\mathbb{Z}^2} \sqrt{3}\,\phi(z_1')\,\chi(z_2'^2)\,|z_1'\rangle\ . \tag{29}$$

One immediately sees that the corresponding integral for the expectation value separates.

4 Approximation of the momentum operator

As mentioned in section 2, in the polymer representation a momentum operator cannot be defined. One may ask, in which sense the Schrödinger momentum operator can be approximated within the polymer representation. Consider, for instance, the coherent Schrödinger state

$$\psi(x) = (\pi d^2)^{-\frac{1}{4}} \exp\left(-\frac{(x-x_0)^2}{2d^2} + ip_0(x-x_0)\right) , \qquad (30)$$

where d is a length scale, such that the inverse of d is proportional to the uncertainty in p. The expectation value for p in this state is p_0, the expectation value of p^2 is $\langle p^2\rangle = p_0^2 + \frac{1}{d^2}$. For $\beta^2\langle p^2\rangle \ll 1$ the operator (see [1])

$$p_\beta = \frac{i}{2\beta}(V(\beta) - V(-\beta)) \qquad (31)$$

is an approximation of the standard Schrödinger momentum operator. In particular, the expectation value of p_β in the coherent state above is

$$\begin{aligned} (\psi, p_\beta\psi) &= \frac{i}{2\beta}\, e^{-\frac{\beta^2}{4d^2}} \left(e^{-ip_0\beta} - e^{ip_0\beta}\right) \\ &= p_0\left(1 + \mathcal{O}(\langle p^2\rangle\beta^2)\right) \ . \end{aligned} \qquad (32)$$

For a given β we may now consider the expectation value of p_β in the polymer state

$$\Psi_\beta = \beta^{\frac{1}{2}} \sum_{z\in\mathbb{Z}} \psi(\beta z)|\beta z\rangle. \qquad (33)$$

and obtain the approximation

$$|(\Psi_\beta, p_\beta\Psi_\beta) - (\psi, p\psi)| \sim \mathcal{O}(p_0\langle p^2\rangle\beta^2) \ . \qquad (34)$$

The difficulty is that for every choice of β one has to use a different polymer state. It is impossible to find a polymer state which approximates the expectation value of the momentum for all sufficiently small values of β. This is due to the fact that the polymer representation is not weakly continuous in the parameter β. It is however possible, as explicitly shown in this paper, to find approximations for any finite set of β's. For instance, let $\beta_1, \beta_2 \ll \langle p^2 \rangle^{\frac{1}{2}}$ with β_1/β_2 irrational. Then an approximating polymer state is

$$\Psi_{\beta_1\beta_2} = (\beta_1^2 + \beta_2^2)^{\frac{1}{2}} \sum_{z_1, z_2 \in \mathbb{Z}} \psi(\beta_1 z_1 + \beta_2 z_2)\, \chi_\lambda \left((\beta_2 z_1 - \beta_1 z_2)^2 \right) \ |\beta_1 z_1 + \beta_2 z_2\rangle \ , \tag{35}$$

where we may choose

$$\chi_\lambda(|z|^2) = \sqrt{\frac{\lambda}{\pi}}\, e^{-\lambda^2 |z|^2} \tag{36}$$

with $\lambda < \langle p^2 \rangle^{\frac{1}{2}}$.

5 Conclusions

Given any state of a quantum mechanical particle in the Schrödinger representation we constructed a net of states in the polymer representation of the Weyl algebra such that the expectation values of all elements of the Weyl algebra converge pointwise to the expectation values in the given state. The existence of such a net follows from Fell's Theorem (density of the states of one faithful representation in the set of all states with respect to the weak-*-topology on the dual of a C*-algebra), but the proof of the theorem is not constructive and therefore does not amount to an explicit construction. Previous explicit approximations of states in the Schrödinger representations were in terms of linear functionals which could not be interpreted as expectation values of states in the polymer representation.

As a byproduct we proved that pure states in the Schrödinger representation can be approximated by pure states in the polymer representation. This goes beyond the assertion of Fell's Theorem.

Observables which can only be defined in the Schrödinger representation (as the momentum operator discussed in the previous section) have first to be approximated by linear combinations of Weyl operators (in the sense of expectation values and, possibly, uncertainties). For a finite number of these approximations one then can find polymer states with approximately equal expectation values (and uncertainties).

It depends on the problem under investigation whether the proven convergence is strong enough. Since the representations are inequivalent, a uniform approximation is not possible. In particular, the question whether the spectrum of an observable is discrete or continuous depends on the equivalence class of the representation (as exemplified by the position operator). Moreover, it is not possible to replace the net of states by a sequence. Namely, given any sequence Ψ_n of normalized wave functions in the polymer Hilbert space, the expectation value of $W(\alpha, \beta)$ vanishes for all n up to a countable set of values for β. In the Schrödinger representation, however, the expectation value in any given state must be near to unity for small values of α and β.

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